

An Overview of Components for Scientific Computing and Introduction to the Common Component Architecture

CCA Forum Tutorial Working Group

http://www.cca-forum.org/tutorials/ tutorial-wg@cca-forum.org



















Goals of This Module

- Introduce basic concepts and vocabulary of component-based software engineering
- Highlight the special demands of high-performance scientific computing on component environments
- Introduce some terminology and concepts from the Common Component Architecture
- Provide a unifying context for the remaining talks
 - For those attending the extended CCA tutorial



Motivation: Modern Scientific Software Engineering Challenges

Productivity

- Time to first solution (prototyping)
- Time to solution ("production")
- Software infrastructure requirements ("other stuff needed")

Complexity

- Increasingly sophisticated models
- Model coupling multi-scale, multi-physics, etc.
- "Interdisciplinarity"

Performance

- Increasingly complex algorithms
- Increasingly complex computers
- Increasingly demanding applications



Motivation: For Library Developers

- People want to use your software, but need wrappers in languages you don't support
 - Many component models provide language interoperability
- Discussions about standardizing interfaces are often sidetracked into implementation issues
 - Components separate interfaces from implementation
- You want users to stick to your published interface and prevent them from stumbling (prying) into the implementation details
 - Most component models actively enforce the separation



Motivation: For Application Developers and Users

- You have difficulty managing multiple third-party libraries in your code
- You (want to) use more than two languages in your application
- Your code is long-lived and different pieces evolve at different rates
- You want to be able to swap competing implementations of the same idea and test without modifying any of your code
- You want to compose your application with some other(s) that weren't originally designed to be combined



Some Observations About Software...

- "The complexity of software is an essential property, not an accidental one." [Brooks]
 - We can't get rid of complexity
- "Our failure to master the complexity of software results in projects that are late, over budget, and deficient in their stated requirements." [Booch]
 - We must find ways to manage it



More Observations...

- "A complex system that works is invariably found to have evolved from a simple system that worked... A complex system designed from scratch never works and cannot be patched up to make it work." [Gall]
 - Build up from simpler pieces
- "The best software is code you don't have to write" [Jobs]
 - Reuse code wherever possible



Component-Based Software Engineering

 CBSE methodology is emerging, especially from business and internet areas

Software productivity

- Provides a "plug and play" application development environment
- Many components available "off the shelf"
- Abstract interfaces facilitate reuse and interoperability of software

Software complexity

- Components encapsulate much complexity into "black boxes"
- Plug and play approach simplifies applications
- Model coupling is natural in component-based approach

Software performance (indirect)

 Plug and play approach and rich "off the shelf" component library simplify changes to accommodate different platforms

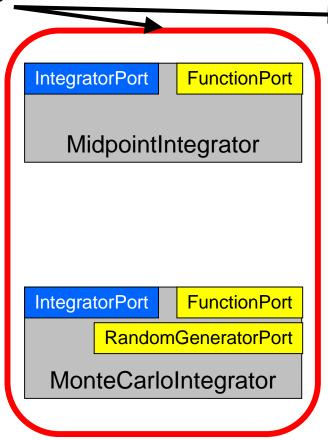


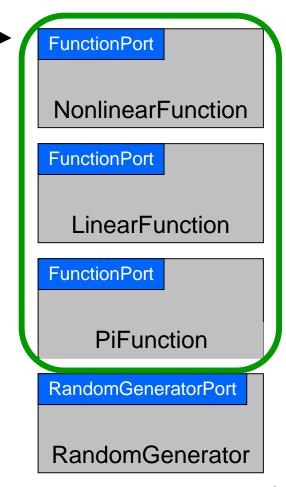
A Simple Example: Numerical Integration Components

Interoperable components (provide same interfaces)

GoPort IntegratorPort

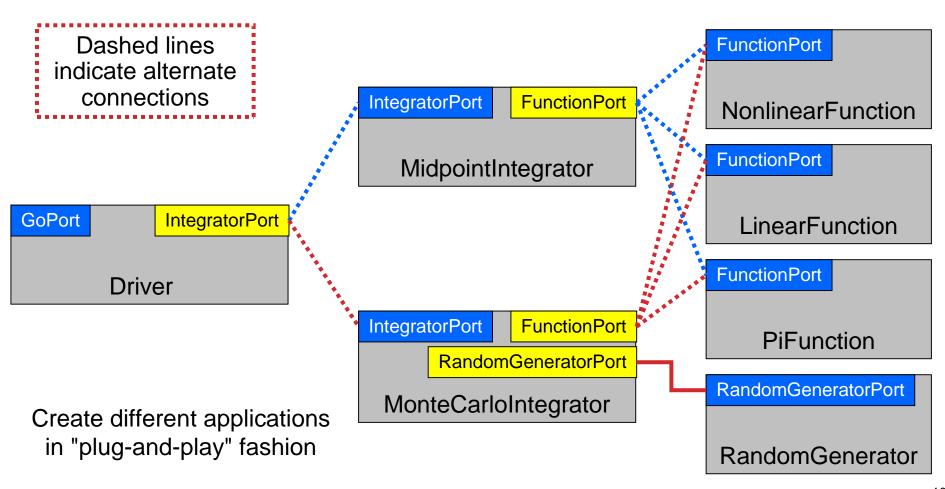
Driver







Many Applications are Possible...





The "Sociology" of Components

- Components need to be shared to be truly useful
 - Sharing can be at several levels
 - Source, binaries, remote service
 - Various models possible for intellectual property/licensing
 - Components with different IP constraints can be mixed in a single application
- Peer component models facilitate collaboration of groups on software development
 - Group decides overall architecture and interfaces
 - Individuals/sub-groups create individual components

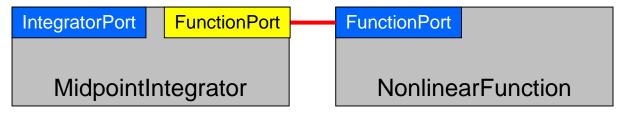


Who Writes Components?

- "Everyone" involved in creating an application can/should create components
 - Domain scientists as well as computer scientists and applied mathematicians
 - Most will also use components written by other groups
- Allows developers to focus on their interest/specialty
 - Get other capabilities via reuse of other's components
- Sharing components within scientific domain allows everyone to be more productive
 - Reuse instead of reinvention
- As a unit of publication, a well-written and –tested component is like a high-quality library
 - Should receive same degree of recognition
 - Often a more appropriate unit of publication/recognition than an entire application code



CCA Concepts: Components



- Components are a unit of software composition
 - Composition is based on interfaces (ports)
- Components provide/use one or more ports
 - A component with no ports isn't very interesting
 - Components interact via ports; implementation is opaque to the outside world
- Components include some code which interacts with the CCA framework
- The granularity of components is dictated by the application architecture and by performance considerations
- Components are peers
 - Application architecture determines relationships



What is a Component Architecture?

- A set of standards that allows:
 - Multiple groups to write units of software (components)...
 - And have confidence that their components will work with other components written in the same architecture
- These standards define...
 - The rights and responsibilities of a component
 - How components express their interfaces
 - The environment in which are composed to form an application and executed (framework)
 - The rights and responsibilities of the framework

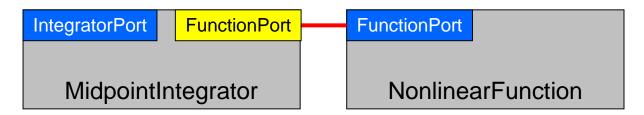


CCA Concepts: Frameworks

- The framework provides the means to "hold" components and compose them into applications
 - The framework is often application's "main" or "program"
- Frameworks allow exchange of ports among components without exposing implementation details
- Frameworks provide a small set of standard services to components
 - BuilderService allow programs to compose CCA apps
- Frameworks may make themselves appear as components in order to connect to components in other frameworks
- Currently: specific frameworks support specific computing models (parallel, distributed, etc.).
 Future: full flexibility through integration or interoperation



CCA Concepts: Ports



- Components interact through well-defined interfaces, or ports
 - In OO languages, a port is a class or interface
 - In Fortran, a port is a bunch of subroutines or a module
- Components may provide ports implement the class or subroutines of the port ("Provides" Port
- Components may <u>use</u> ports <u>call</u> methods or subroutines in the port (<u>"Uses" Port</u>)
- Links denote a procedural (caller/callee) relationship, not dataflow!
 - e.g., FunctionPort could contain: evaluate(in Arg, out Result)



Interfaces, Interoperability, and Reuse

- Interfaces define how components interact...
- Therefore interfaces are key to interoperability and reuse of components
- In many cases, "any old interface" will do, but...
- General plug and play interoperability requires multiple implementations providing the same interface
- Reuse of components occurs when they provide interfaces (functionality) needed in multiple applications



Designing for Reuse, Implications

- Designing for interoperability and reuse requires "standard" interfaces
 - Typically domain-specific
 - "Standard" need not imply a formal process, may mean "widely used"
- Generally means collaborating with others
- Higher initial development cost (amortized over multiple uses)
- Reuse implies longer-lived code
 - thoroughly tested
 - highly optimized
 - improved support for multiple platforms



Relationships: Components, Objects, and Libraries

- Components are typically discussed as objects or collections of objects
 - Interfaces generally designed in OO terms, but...
 - Component internals need not be OO
 - OO languages are not required
- Component environments can enforce the use of published interfaces (prevent access to internals)
 - Libraries can not
- It is possible to load several instances (versions) of a component in a single application
 - Impossible with libraries
- Components must include some code to interface with the framework/component environment
 - Libraries and objects do not



Domain-Specific Frameworks vs Generic Component Architectures

Domain-Specific

- Often known as "frameworks"
- Provide a significant software infrastructure to support applications in a given domain
 - Often attempts to generalize an existing large application
- Often hard to adapt to use outside the original domain
 - Tend to assume a particular structure/workflow for application
- Relatively common

Generic

- Provide the infrastructure to hook components together
 - Domain-specific infrastructure can be built as components
- Usable in many domains
 - Few assumptions about application
 - More opportunities for reuse
- Better supports model coupling across traditional domain boundaries
- Relatively rare at present
 - Commodity component models often not so useful in HPC scientific context



Special Needs of Scientific HPC

- Support for legacy software
 - How much change required for component environment?
- Performance is important
 - What overheads are imposed by the component environment?
- Both parallel and distributed computing are important
 - What approaches does the component model support?
 - What constraints are imposed?
 - What are the performance costs?
- Support for languages, data types, and platforms
 - Fortran?
 - Complex numbers? Arrays? (as first-class objects)
 - Is it available on my parallel computer?



Commodity Component Models

- CORBA, COM, Enterprise JavaBeans
 - Arise from business/internet software world
- Componentization requirements can be high
- Can impose significant performance overheads
- No recognition of tightly-coupled parallelism
- May be platform specific
- May have language constraints
- May not support common scientific data types



What is the CCA? (User View)

- A component model specifically designed for high-performance scientific computing
- Supports both parallel and distributed applications
- Designed to be implementable without sacrificing performance
- Minimalist approach makes it easier to componentize existing software



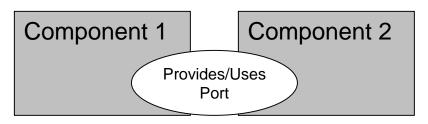
What is the CCA? (2)

- Components are peers
- Not just a dataflow model
- A tool to enhance the productivity of scientific programmers
 - Make the hard things easier, make some intractable things tractable
 - Support & promote reuse & interoperability
 - Not a magic bullet

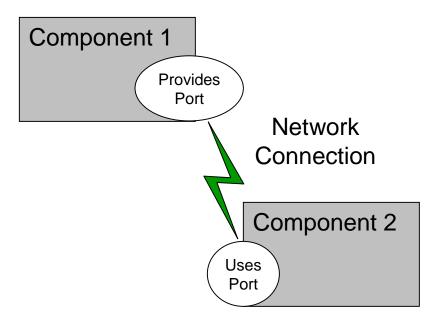


Importance of Provides/Uses Pattern for Ports

- Fences between components
 - Components must declare both what they provide and what they use
 - Components cannot interact until ports are connected
 - No mechanism to call anything not part of a port
- Ports preserve high performance direct connection semantics...
- ...While also allowing distributed computing



Direct Connection





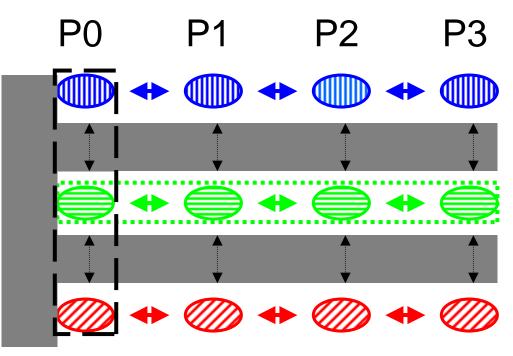
CCA Concepts: "Direct Connection" Maintains Local Performance

- Calls between components equivalent to a C++ virtual function call: lookup function location, invoke it
 - Cost equivalent of ~2.8 F77 or C function calls
 - ~48 ns vs 17 ns on 500 MHz Pentium III Linux box
- Language interoperability can impose additional overheads
 - Some arguments require conversion
 - Costs vary, but small for typical scientific computing needs
- Calls within components have no CCA-imposed overhead
- Implications
 - Be aware of costs
 - Design so inter-component calls do enough work that overhead is negligible



CCA Concepts: Framework Stays "Out of the Way" of Component Parallelism

- Single component multiple data (SCMD) model is component analog of widely used SPMD model
- Each process loaded with the same set of components wired the same way
- Different components in same process "talk to each" other via ports and the framework
- Same component in different processes talk to each other through their favorite communications layer (i.e. MPI, PVM, GA)



Components: Blue, Green, Red

Framework: Gray

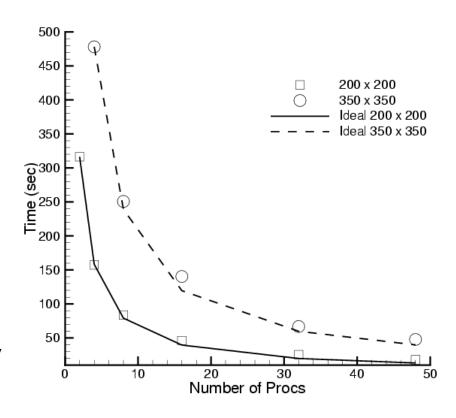
MCMD/MPMD also supported

Other component models ignore parallelism entirely



Scalability of Scientific Data Components in CFRFS Combustion Applications

- Investigators: S. Lefantzi, J. Ray, and H. Najm (SNL)
- Uses GrACEComponent, CvodesComponent, etc.
- Shock-hydro code with no refinement
- 200 x 200 & 350 x 350 meshes
- Cplant cluster
 - 400 MHz EV5 Alphas
 - 1 Gb/s Myrinet
- Negligible component overhead
- Worst perf: 73% scaling efficiency for 200x200 mesh on 48 procs

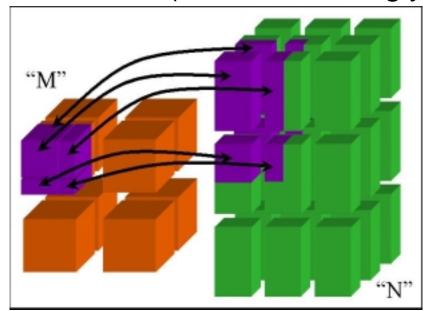


Reference: S. Lefantzi, J. Ray, and H. Najm, Using the Common Component Architecture to Design High Performance Scientific Simulation Codes, *Proc of Int. Parallel and Distributed Processing Symposium*, Nice, France, 2003, accepted.



CCA Concepts: MxN Parallel Data Redistribution

- Share Data Among Coupled Parallel Models
 - Disparate Parallel Topologies (M processes vs. N)
 - e.g. Ocean & Atmosphere, Solver & Optimizer...
 - e.g. Visualization (Mx1, increasingly, MxN)

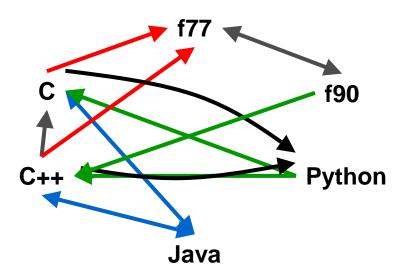


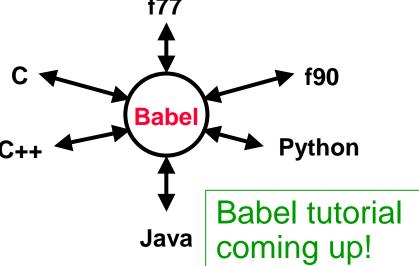
Research area -- tools under development



CCA Concepts: Language Interoperability

- Existing language interoperability approaches are "pointto-point" solutions
- Babel provides a unified approach in which all languages are considered peers
- Babel used primarily at interfaces





Few other component models support all languages and data types important for scientific computing



What the CCA isn't...

- CCA doesn't specify who owns "main"
 - CCA components are peers
 - Up to application to define component relationships
 - "Driver component" is a common design pattern
- CCA doesn't specify a parallel programming environment
 - Choose your favorite
 - Mix multiple tools in a single application
- CCA doesn't specify I/O
 - But it gives you the infrastructure to create I/O components
 - Use of stdio may be problematic in mixed language env.
- CCA doesn't specify interfaces
 - But it gives you the infrastructure to define and enforce them
 - CCA Forum supports & promotes "standard" interface efforts
- CCA doesn't require (but does support) separation of algorithms/physics from data



What the CCA is...

- CCA is a specification for a component environment
 - -Fundamentally, a design pattern
 - -Multiple "reference" implementations exist
 - -Being used by applications
- CCA increases productivity
 - -Supports and promotes software interopability and reuse
 - -Provides "plug-and-play" paradigm for scientific software
- CCA offers the flexibility to architect your application as you think best
 - -Doesn't dictate component relationships, programming models, etc.
 - -Minimal performance overhead
 - -Minimal cost for incorporation of existing software
- CCA provides an environment in which domain-specific application frameworks can be built
 - -While retaining opportunities for software reuse at multiple levels



Review of CCA Terms & Concepts

Ports

- Interfaces between components
- Uses/provides model

Framework

Allows assembly of components into applications

Direct Connection

Maintain performance of local inter-component calls

Parallelism

Framework stays out of the way of parallel components

MxN Parallel Data Redistribution

Model coupling, visualization, etc.

Language Interoperability

Babel, Scientific Interface Definition Language (SIDL)



Summary

- Components are a software engineering tool to help address software productivity and complexity
- Important concepts: components, interfaces, frameworks, composability, reuse
- Scientific component environments come in "domain specific" and "generic" flavors
- Scientific HPC imposes special demands on component environments
 - Which commodity tools may have trouble with
- The Common Component Architecture is specially designed for the needs of HPC